A NEW APPROACH TO NUMERICAL ALGORITHMS

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Introduction

- In this paper we developed a new Lanczos algorithm on the Grassmann manifold.
- This work comes in the wake of the article by A. Edelman, T. A. Arias and S. T. Smith, *"The geometry of algorithms with orthogonality constraints"*

Introduction

- The Grassmann and Stiefel manifolds are based on orthogonality constraints
- The Lanczos method and the conjugate gradients method are closely related
- One of the main problems of the Lanczos method is the loss of orthogonality

Numerical linear algebra problems

- The problem of computing eigenvalues, eigenvectors and invariant subspaces is always present in areas as diverse as Engineering, Physics, Computer Sciences and Mathematics.
- Lately, it has been verified that the iterations of eigenvalues and eigenvectors problems are best analyzed in some special spaces.
- A bridge between the geometry of the abstract spaces and the well known algorithms of numerical linear algebra.

Optimization Problem

- The optimization problem of the estimative of the invariant subspaces is made explicit with a geometric approach.
- However a geometrical treatment on the Grassmann manifold appropriate for numerical linear algebra is not present in standard references.

Grassmann Manifold

- Gr(p,n) – Grassmann Manifold :
  p – dimensional subspaces in $\mathbb{R}^n$
- Identify matrix algorithms that induce iterations on the Grassmann manifold
- Translate abstractly defined Grassmannian algorithms into tractable numerical algorithms
- Use suitable matrix representations that facilitate convergence analysis

Iterations on the Grassmann Manifold

- One possible way to represent numerically an element $\mathcal{Y}$ of Gr(p,n) consists of specifying an $n \times p$ full column rank matrix Y whose columns span the space $\mathcal{Y}$, and we can write
  $$\mathcal{Y} = span(Y)$$
- $\mathcal{Y}$ is called the column space of Y
- The set of all the matrices that have the same column space is a fiber over Y

Iterations on the Grassmann Manifold

- We have an iteration on the Grassmann Manifold if a fiber is mapped into a fiber
- The concept of the fiber bundle structure allows us to describe the relationship between subspaces and matrices representations

Lanczos on the Grassmann manifold

- The Lanczos algorithm is a method for computing some eigenvalues of a large symmetric matrix A and their eigenvectors
- The idea consists in building a sequence of nested subspaces span $x, Ax, A^2x, \ldots$ and solving the eigenproblem reduced to these subspaces

Algorithm Grassmann-Lanczos (GL)

Let A be an symmetric matrix $n \times n$
Consider $\mathcal{Y}$ an p-dimensional subspace of $\mathbb{R}^n$ i.e.,

$$\mathcal{Y} \in \mathrm{Gr}(p,n)$$

The algorithm produce a sequence of subspaces

$$\begin{aligned} \mathrm{Gr}(p,n) &\to \mathrm{Gr}(p,n) \\ \mathcal{Y} &\mapsto \mathcal{Y}_+ \end{aligned}$$

Algorithm Grassmann-Lanczos (GL)

1. Pick an orthonormal matrix $Y, n \times p$, being $\mathcal{Y} = \mathrm{span}(Y)$
2. Create an orthonormal basis Q for the Krylov subspace
   $$\mathcal{K}_m(Y) = span \;\; Y, AY, \ldots, A^{m-1}Y$$
3. Calculate the matrix Rayleigh quotient $M = Q^T AQ$ that represents the projection of A into $\mathcal{K}_m(Y)$
4. Calculate X, an orthonormal basis for the p- dimensional dominated eigenspace of M
5. Let $\mathcal{Y}_+$ be the span of QX

Algorithm Grassmann-Lanczos (GL)

- Doesn't have a function that maps fibers to fibers
- The algorithm is defined as a mapping
- This algorithm is well - defined

$$\mathrm{Gr}(p,n) \rightarrow \mathrm{Gr}(p,n)$$

Conclusion and Future Work

- This paper offers a new approach to the Lanczos algorithm
- Lanczos algorithm is a very competitive method whose main problem is the loss of orthogonality, but the introduction of Grassmann manifolds seems to solve this problem
- This method might be easily implemented by blocks

Conclusion and Future Work

- We believe that this method is competitive in sequential computation, and also in parallel computing
- Until now, as far as we know, people haven't though of Lanczos as a subspace iteration
- We intend to obtain new convergence results and make extensive comparisons with other Grassmannian methods

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Thank you
Teşekkür ederim
Obrigado